

## Nuclear quadrupole resonance and x-ray investigation of the structure of Na<sub>2/3</sub> CoO<sub>2</sub>

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### Abstract

We have synthesized various samples of the  $x=2/3$  phase of sodium cobaltate Na<sub>x</sub> CoO<sub>2</sub> and performed x-ray powder diffractions spectra to compare the diffraction with the structure proposed previously from NMR and nuclear quadrupole resonance (NQR) experiments. Rietveld analyses of the data are found in perfect agreement with those and confirm the concentration  $x=2/3$  obtained in the synthesis procedure. They even give indications on the atomic displacements of Na inside the unit cell. The detailed NQR data allow us to identify the NQR transitions and electric field gradient parameters for four cobalt sites and three Na sites. The spin-lattice and spin-spin relaxation rates are found much smaller for the nonmagnetic Co<sup>3+</sup> sites than for the magnetic sites on which the holes are delocalized. The atomic ordering of the Na layers is therefore at the source of this ordered distribution of cobalt charges. The method used here to resolve the Na ordering and the subsequent Co charge order can be used valuably for similar structural determinations for various phases with  $x>0.45$  for which Na ordering has been established. © 2009 The American Physical Society.

<http://dx.doi.org/10.1103/PhysRevB.80.224106>

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